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Photocurrent calculations in semiconductors using Kronig-Penney model

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Abstract : Photoemission calculations have been done using the Kronig-Penney model from band state (Fermi level) of semiconductors silicon and gallium arsenide. For the evaluation of photocurrent the initial state wavefunction used is the one deduced by Thapa and Kar [*Indian J Pure Appl. Phys.* **26** 620 (1988)] [1].

Keywords : Photoemission, semiconductors, Kronig-Penney model

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The existence of surface states on semiconductor surfaces was experimentally verified by using the angle integrated photoemission [2]. Moreover their existence is obvious through the pinning of the Fermi level at the surface. However, the semiconductor surfaces are more complex than metal surfaces for the reason that semiconductor surfaces reconstruct [3]. The presence of these reconstructions and atomic displacements on semiconductor surfaces makes the studies of electronic structure a very interesting topic. Of the various tools and techniques, angle resolved photoemission studies has also been widely used in understanding the surface states of semiconductors. Various type of structural models of semiconductors have been proposed [4]. But in this short report, we will be mainly concerned with the photoemission studies by adopting a simple calculational procedure which will be applied to the case of silicon and gallium arsenide.

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For photoemission calculations the current density may be written with the help of the golden rule expression [5] as

$$\frac{dj(E)}{d\Omega} = \frac{2\pi}{\hbar}\sum \left|\langle \psi_f |\Delta| \psi_i \rangle\right|^2 \delta(E-E_f)\,\delta(E_f - E_i - \hbar\omega)$$

$$\times f_0(E-\hbar\omega)[1-f_0(E)], \tag{1}$$

where $|\psi_i\rangle\left(|\psi_f\rangle\right)$ refer to the initial (final state), $\Delta = (e/2\,mc)(\boldsymbol{A}.\boldsymbol{p} + \boldsymbol{p}.\boldsymbol{A})$, and $\boldsymbol{p}$ being the one-electron momentum operator, $\boldsymbol{A}$ the vector potential of the photon field. Although the one-electron states are treated quite accurately in many photoemission calculations, the variation of the photon fields in the surface region is usually neglected. The model dielectric function which takes into account the bulk, surface and vacuum regions is given [6] by

$$\begin{aligned} \varepsilon(\omega) &\equiv \begin{cases} \varepsilon_1 + i\varepsilon_2, & z \le -a \\ 1 + [1-\varepsilon(\omega)]\frac{z}{a}, & -a \le z \le 0 \\ 1, & z \ge 0. \end{cases} \\ \varepsilon(\omega, z) &= \end{aligned} \tag{2}$$

We have used the Drude-Lorentz model for calculating the frequency dependent dielectric constants which is given by

$$\varepsilon(\omega) = \varepsilon_\infty\left[1 - \frac{\omega_p^2}{\omega(\omega + i\gamma_1)}\right] + \frac{(\varepsilon_0 - \varepsilon_\infty)\omega_0^2}{\left(\omega_0^2 - \omega^2 - \imath\gamma_2\omega\right)}. \tag{3}$$

In eq. (3) above, ε_0 and ε_∞ are the static and high frequency dielectric constants. By using the appropriate values of constants ε_0, ε_∞, γ_1, γ_2 *etc* respectively for silicon and gallium arsenide, the real and imaginary parts of $\varepsilon(\omega)$ were calculated by using eq. (3) which were then applied to eq. (2) for computing the fields.

Using the electromagnetic field for *p*-polarized radiation, we calculate the photoemission cross section by evaluating the matrix element :

$$\langle \psi_f |\Delta| \psi_i \rangle = \int_{-\infty}^{\infty} \psi_f^*(z)\Delta\psi_i(z)\,dz$$

$$= \int_{-\infty}^{\infty}\left[\psi_f^*(z)A_\omega(z)\frac{d\psi_i}{dz} + \frac{1}{2}\psi_f^*\frac{dA_\omega}{dz}\psi_i(z)\right]dz, \tag{4}$$

where [6]

$$A_\omega(z) = \begin{cases} A_1^*, & z \le -a \\ \dfrac{a\varepsilon(\omega)}{A_1[1-\varepsilon(\omega)]z + a}, & -a \le z \le 0 \\ A_1\varepsilon(\omega), & z \ge 0. \end{cases} \tag{5}$$

A_1 is a constant whose value depends on the angle of the incident radiation (θ_i) and its frequency (ω) and dielectric constants $\varepsilon(\omega)$. In the surface region ($-a \le z \le 0$), the dielectric

function is linearly interpolated between the vacuum and the bulk values. $\psi_f(z)$ in eq. (4) is the free-electron final-state wavefunction given by

$$\psi_f(z) = \left(\frac{1}{2\pi q}\right)^{\frac{1}{2}} \frac{2q}{q+k_f} e^{ik_f z}, \qquad z<0$$

$$= \left(\frac{1}{2\pi q}\right)^{\frac{1}{2}} \left[e^{iqz} + \left(\frac{q-k_f}{q+k_f}\right) e^{-iqz}\right], \qquad z>0 \tag{6}$$

where $k_f^2 = 2E_f$, $q^2 = 2(E_f - V_0)$ and $E_f = E_i + \hbar\omega$.

To evaluate the initial state wavefunction $\psi_i(z)$, one solves the one-dimensional Schroedinger's equation

$$\frac{d^2\psi(z)}{dz^2} + k_i^2(z) = -2V(z)\psi(z), \tag{7}$$

where $k_i^2 = 2E_i$ and $V(z)$ is the δ-function potential of the Kronig-Penney (K–P) model.

Let $\phi(z)$ denote the Bloch wavefunction deep inside the metal and $\phi^*(z)$ the time reversal of $\phi(z)$. The eigenfunction in the semi-infinite solid ($z < 0$) was chosen [7] to have the form $\psi_i(z) = \phi(z) - P\phi^*(z)$, where P is the reflection coefficient obtained by matching the wavefunction and its derivative at $z = 0$. One can then show [1] that the initial state wavefunction for $z < 0$ may be written as

$$\psi_i(z) = \left(1 - iPe^{-i\delta}\sin\delta\right)e^{ik_i z} - \left(P - ie^{i\delta}\sin\delta\right)e^{-ik_i z}, \tag{8}$$

where $\cot\delta = \dfrac{k_i}{g}$, g being the strength of the potential. The initial-state wavefunction outside the metal ($z > 0$) is

$$\psi_i = Te^{-\chi z}, \tag{9}$$

T being the transmission coefficient across the boundary plane and $\chi^2 = 2(V_0 - E_i)$, where V_0 is the surface step potential. From the matching conditions at $z = 0$, one can easily deduce the values of P and T in eqs. (8) and (9) and write the most explicit form of initial state wavefunction $|\psi_i\rangle$. The photoemission cross section was obtained *via*

$$\frac{d\sigma}{d\Omega} = \frac{k^2}{\omega}\sum\left|\langle\psi_f|\Delta|\psi_i\rangle\right|^2. \tag{10}$$

The matrix element $I = \langle\psi_f|\Delta|\psi_i\rangle$ in eq. (10) can be expanded as

$$I = \int_{-\infty}^{-a}\psi_f^* A_\omega(z)\frac{d\psi_i}{dz}dz + \int_{-a}^{0}\psi_f^* A_\omega\frac{d\psi_i}{dz}dz + \frac{1}{2}\int_{-a}^{0}\psi_f^*\frac{dA_\omega(z)}{dz}\psi_i dz$$

$$+ \int_0^{\infty}\psi_f^* A_\omega(z)\frac{d\psi_i}{dz}dz. \tag{11}$$

In calculating the photocurrent, these integrals were evaluated analytically wherever possible, or numerically by developing a FORTRAN programme. To ensure the convergence, a factor of $e^{-\alpha|z|}$ (α is the scattering factor) was introduced for $z < 0$ which represents the effect of inelastic collisions.

Since it is strictly a model calculation, we have used the same set of data (in atomic units) both for silicon and gallium arsenide. The data used are :

Fermi level (E_F) = 0.463,

Work function (ϕ) = 0.198,

Surface width (a) = 10,

Height of the potential barrier (V_0) = 0.662,

Strength of the potential barrier (g) = 0.60,

Phase factor (δ) = –0.5776,

Scattering factor (α) = 0.35.

We have chosen the initial state energy (E_i) to lie at the Fermi level. The values of the parameters g, δ and α are chosen arbitrarily to fit in such a way that it can reproduce qualitatively the nature of the photon energy dependence of the square of the field. The reason for this being that the matrix element for photoemission cross section is a quadratic function of the photon field.

In Figure 1, we have shown the plot of photocurrent as a function of photon energy ($\hbar\omega$). For the surface width a = 10 a.u., we find that at $\hbar\omega$ = 12 eV, photocurrent peak is

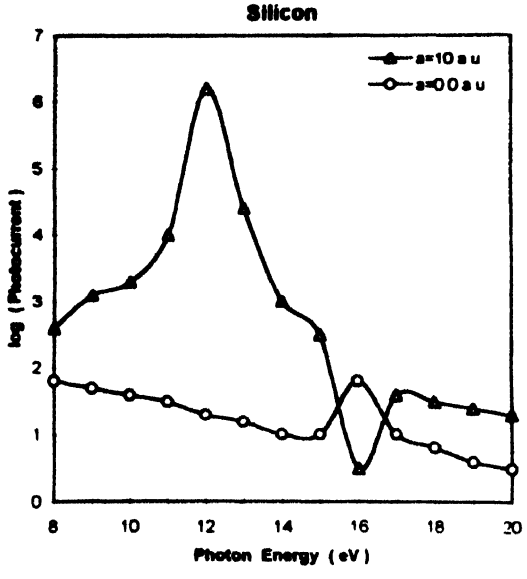

Figure 1. Plots of log (photocurrent) (in arb. units) as a function of photon energy for silicon for surface widths a = 10.0 a.u. and 0.0 using the Drude-Lorentz dielectric model.

maximum. It shows a minimum at $\hbar\omega = 16$ eV followed by a small hump at 17 eV. Further increase of $\hbar\omega$ causes the photocurrent to decay towards a minimum value. We have taken the plasmon energy ($\hbar\omega_p$) of silicon to be 16 eV. Interesting feature that is seen here in the case of silicon is that photocurrent data showed behaviour similar at least qualitatively with the earlier results [8] when fields were calculated by using the experimentally measured dielectric constants. For example, the maxima in photocurrent was obtained at $\hbar\omega < \hbar\omega_p$ *i.e.*, at 12 eV photon energy followed by a minima occurring at $\hbar\omega = \hbar\omega_p$. For the case of narrow surface width ($a = 0.0$) the behaviour in photocurrent is completely different. We find that a peak of low height in photocurrent occurred but at plasmon energy of silicon. This is quite different behaviour obtained than with the one [8] calculated by using the experimentally determined dielectric constants.

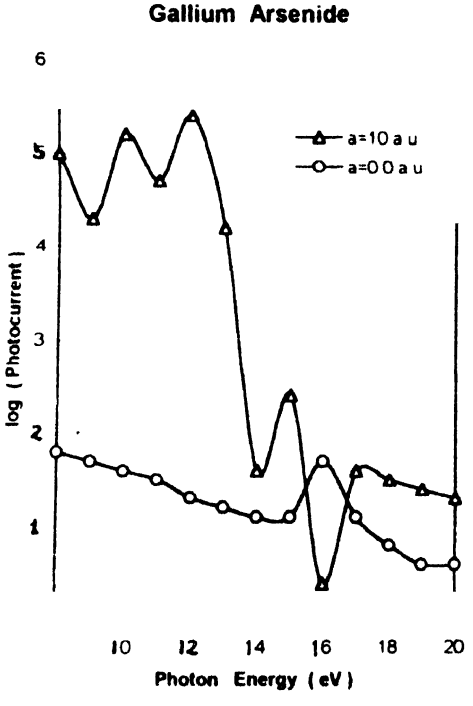

Figure 2. Plots of log (photocurrent) (in arb. units) as a function of photon energy for gallium arsenide for surface widths $a = 10.0$ a.u. and 0.0 using the Drude-Lorentz dielectric model.

In Figure 2, the plot of photocurrent as a function of photon frequency in the case of gallium arsenide is shown for two different surface widths $a = 10.0$ a.u. and $a = 0.0$ respectively, but with the same values of Kronig-Penney parameters as were used in the case of silicon. The photocurrent structures of gallium arsenide data showed three peaks at $\hbar\omega = 10$, 12 and 15 eV respectively but showing a minima at $\hbar\omega = 16$ eV (the assumed plasmon energy of gallium arsenide). Another hump in the photocurrent is seen at 17 eV beyond which the photocurrent decreases gradually. The photocurrent data for

narrow surface width ($a = 0.0$) is found to be similar as in the case of silicon. The reason for this being that for $a = 0.0$, both silicon and gallium arsenide had almost same values of dielectric constants as calculated by using the Drude-Lorentz formula.

Photoemission is considered basically to be a surface effect. It is dependent mainly on the spatial variation of the photon field vector at the surface region. We find therefore that in the case of silicon, the model dielectric response function of Drude-Lorentz seems to work quite fittingly for values of photon energies below and above the plasmon energy. However, strikingly different behaviour is seen in photocurrent in the case of gallium arsenide. For example, we find three peaks in photocurrent for $\hbar\omega < \hbar\omega_p$ a result seen quite different from that of silicon [8] and other metals like aluminium [9], palladium [10], tungsten [8] *etc.* The reason for this may be attributed to the fact that the Drude-Lorentz model for calculating the dielectric constants is not applicable to the case of gallium arsenide. The other reason for the occurrence of such peaks may be that for $\hbar\omega < \hbar\omega_p$ the photon field vector $A_\omega(z)$ as deduced by using the model of Bagchi and Kar [6] is not applicable to the case of compound semiconductor. We cannot rule out the weakness of the K–P model potential as used by Thapa and Kar [1] for deducing the initital state wavefunction ψ_i. The effect of the surface was not taken into consideration while formulating ψ_i for a semi-infinite solid. However, the occurrence of peaks at $\hbar\omega < \hbar\omega_p$ both for silicon and gallium arsenide can be attributed to the spatial variation of vector potential. Lapeyre and Anderson [11] had also experimentally found the existence of surface state in gallium arsenide from the constant initial state spectroscopy. The complicated line shapes in their measurement for the surface states were not fully understood. However, the conclusion found in their measurement was that the photoemission intensity was strongly a polarization dependent.

Though we have not taken into consideration the effect of the type of semiconductor, density *etc*, however, we find that in the case of semiconductors, the spatial dependence of vector potential is an essential ingredient in photoemission calculations. Instead of using the simple type of dielectric formula like that of Drude-Lorentz type, it would be more realistic if one can employ the method as developed by Cappellini [12] *et al* which is specifically defined only for the semiconductors. Further, the inclusion of structure into this type of calculations will enable one to compare the data with experiment in a more appropriate way. For example, a detailed study of photoemission from semiconductor gallium arsenide by using the one-step model of photoemission had been done by Schattke [13]. He had used the Green function-formalism to the valence states in LCAO basis by taking photon field vector as constant in dipole approximation. The photoemission data for the ideal gallium arsenide surface agreed well with the experimental data.

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